

Bethe Ansatz Equations of XXZ Model and q -Sturm-Liouville Problems

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Abstract

In this article we have discovered a close relationship between the (algebraic) Bethe Ansatz equations of the spin s XXZ model of a finite size and the q -Sturm-Liouville problem. We have demonstrated that solutions of the Bethe Ansatz equations give rise to the polynomial solutions of a second order q -difference equation in terms of Askey-Wilson operator. The more general form of Bethe Ansatz equations and the mathematical problems relevant to the physics of XXZ model are discussed. Furthermore, the similar correspondence between Bethe Ansatz equations of XXX model and the Sturm-Liouville type difference equation in terms of Wilson operator has also been found.

2000 MSC: 33C45, 33D45, 39A13.

1999 PACS: 02.30Gp, 05.50.+q, 75.10.Jm.

Key words: Askey-Wilson operator, Sturm-Liouville type difference equation, Bethe Ansatz equations, XXZ model, XXX model.

1 Introduction

Among the many one-dimensional integrable quantum spin chains the XXZ spin chain is an important and renowned one. It corresponds to the 6-vertex model in the 2-dimensional solvable statistical mechanics. In particular, the XXZ Hamiltonian of spin $\frac{1}{2}$ of a finite size $2N$ has been the subject of extensive studies for a long time in the physics community, and in recent years it has been investigated by mathematicians in the areas of mathematical physics and quantum algebras. The one-dimensional $U_q(sl_2(\mathbf{C}))$ -invariant XXZ model of spin $\frac{1}{2}$ of a size $2N$ with the open (Dirichlet) boundary condition is described by the following Hamiltonian [21], [18],

$$H_{\text{XXZ}}^{(o)} = - \sum_{j=1}^{2N-1} (\sigma_j^1 \sigma_{j+1}^1 + \sigma_j^2 \sigma_{j+1}^2 + \Delta \sigma_j^3 \sigma_{j+1}^3) - \frac{q - q^{-1}}{2} (\sigma_1^3 - \sigma_{2N}^3), \quad \Delta := \frac{q + q^{-1}}{2}, \quad (1.1)$$

where σ_n^j are the Pauli matrices acting on the j^{th} site:

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The Hamiltonian $H_{\text{XXZ}}^{(o)}$ defines a linear endomorphism of $\bigotimes^{2N} \mathbf{C}^2$, whose eigenvalue problem has been the main concern for the physical quantities related to the system. In the context of quantum inverse scattering method developed by the Leningrad school in the early eighties (see, for example [8], [17]), the diagonalization problem of the Hamiltonian has been investigated by means of solutions of the following algebraic Bethe Ansatz equations,

$$\left(\frac{\sin(\lambda_k + \frac{1}{2}\eta)}{\sin(\lambda_k - \frac{1}{2}\eta)} \right)^{2N} = \prod_{j \neq k, j=1}^n \frac{\sin(\lambda_k + \lambda_j + \eta) \sin(\lambda_k - \lambda_j + \eta)}{\sin(\lambda_k + \lambda_j - \eta) \sin(\lambda_k - \lambda_j - \eta)}, \quad 1 \leq k \leq n.$$

In general, for a given positive half-integer s , the theory also provides a similar XXZ Hamiltonian of spin s of a finite size $2N$ with the following form of Bethe Ansatz equations associated to the corresponding Hamiltonian,

$$\left(\frac{\sin(\lambda_k + s\eta)}{\sin(\lambda_k - s\eta)} \right)^{2N} = \prod_{j \neq k, j=1}^n \frac{\sin(\lambda_k + \lambda_j + \eta) \sin(\lambda_k - \lambda_j + \eta)}{\sin(\lambda_k + \lambda_j - \eta) \sin(\lambda_k - \lambda_j - \eta)}, \quad 1 \leq k \leq n. \quad (1.2)$$

For over half a century the Bethe Ansatz has been a very useful tool in obtaining important informations of the XXZ-model in physics literature; but yet there is no systematic study of the mathematical content on the Bethe Ansatz available at this time. In this paper, we establish an explicit connection between the relation (1.2) and q -Sturm-Liouville problem. In fact, we study the Bethe Ansatz equations in a more general setting than (1.2), namely the system of equations

$$\prod_{l=1}^{2N} \frac{\sin(\lambda_k + s_l \eta)}{\sin(\lambda_k - s_l \eta)} = \prod_{j \neq k, j=1}^n \frac{\sin(\lambda_k + \lambda_j + \eta) \sin(\lambda_k - \lambda_j + \eta)}{\sin(\lambda_k + \lambda_j - \eta) \sin(\lambda_k - \lambda_j - \eta)}, \quad 1 \leq k \leq n, \quad (1.3)$$

where s_l 's are $2N$ complex numbers. The mathematical problem is to obtain the solution(s) of the above system of nonlinear equations. The solution of (1.3) will determine the roots of

a polynomial which satisfies a q -difference relation which is a Sturm-Liouville type equation involving the Askey-Wilson operator, as we shall see in §4. For $N = 2$, the system of equations (1.3) is solved by the zeros of the Askey-Wilson polynomials. An interesting physical problem is to understand the large N behavior of solutions of the system of equations (1.3). Such a study is a challenging problem in the area of q -Sturm-Liouville equations. The understanding of the solutions of (1.3) and their limiting distribution will have a profound impact on the physics of statistical mechanics.

As $q \rightarrow 1$, it is known that the XXZ chain of spin s becomes the $sl_2(\mathbf{C})$ -invariant spin s XXX chain of a finite size $L = 2N$ with the periodic condition. The antiferromagnetic spin $\frac{1}{2}$ XXX chain of size L with periodic condition is given by the following Heisenberg XXX Hamiltonian:

$$H_{\text{XXX}} = -J \sum_{j=1}^L (\sigma_j^1 \sigma_{j+1}^1 + \sigma_j^2 \sigma_{j+1}^2 + \sigma_j^3 \sigma_{j+1}^3 - 1), \quad J < 0. \quad (1.4)$$

The above XXX spin chain is a famous integrable model with many applications to solid state physics and statistical mechanics. It was first proposed by Heisenberg in 1928, [11], then solved by Bethe in 1931 [6]. The spectral problem of H_{XXX} can be reduced to the solution of the following Bethe Ansatz equations,

$$\left(\frac{\lambda_k + \frac{i}{2}}{\lambda_k - \frac{i}{2}} \right)^L = \prod_{j=1, j \neq k}^l \frac{\lambda_k - \lambda_j + i}{\lambda_k - \lambda_j - i}, \quad \lambda_k \in \mathbf{C}, \quad k = 1, \dots, l.$$

We shall discuss the above equations subject to certain symmetry conditions imposed on the roots λ_j 's from physical considerations of the ground state of Hamiltonian H_{XXX} . In this situation, the Bethe Ansatz equations are closely connected to a Sturm-Liouville problem involving a Wilson operator. The solution of this problem requires new developments in the theory of Wilson operators. Further mathematical study of those difference equations could enrich our understanding of both the mathematical and physical contents related to the Bethe Ansatz equations of XXX model. This will be the subject of a future work.

An important contribution of this paper is to point out that the Bethe Ansatz equations are variations on nineteenth century work by Heine, Stieltjes and Hilbert. Heine studied polynomial solutions to a second order differential equations

$$\Pi(x) \frac{d^2 y}{dx^2} + \Phi(x) \frac{dy}{dx} + r(x)y = 0. \quad (1.5)$$

In (1.5), Π and Φ are given polynomials of degrees N and $N - 1$. Heine proved that given a nonnegative integer n , there exists at most $\binom{N+n-2}{N-2}$ choices of the polynomial r in (1.5) such that (1.5) has a polynomial solution. Stieltjes continued this research and showed that if we assume that Π and Φ have only real and simple zeros and their zeros interlace, then there are precisely $\binom{N+n-2}{N-2}$ polynomials r which will make (1.5) have a polynomial solution of degree n . For references and details we refer the interested reader to Szegő's book [22], which also treats Hilbert's work on the location of zeros of Jacobi polynomials $P_n^{(\alpha, \beta)}(x)$ when the conditions of orthogonality, namely $\text{Re } \alpha > -1$, $\text{Re } \beta > -1$, and $\alpha + \beta$ real, are not necessarily assumed.

If we denote the zeros of a polynomial solution of (1.5) by x_1, \dots, x_n then when $x = x_k$, for $1 \leq k \leq n$, equation (1.5) becomes

$$\sum_{1 \leq j \leq n, j \neq k} \frac{1}{x_j - x_k} = \frac{\Phi(x_k)}{2\Pi(x_k)}. \quad (1.6)$$

The system of algebraic equations (1.6) is a system of generalized Bethe Ansatz equations. Observe that although the polynomial r does not appear explicitly in the system (1.6), it is used implicitly to show the existence of a polynomial solution to (1.5), hence the zeros of the polynomial y solve (1.6). Conversely if (1.6) has a solution x_1, \dots, x_n , then we set $y(x) = \prod_{k=1}^n (x - x_k)$ and observe that $\Pi(x)y'' + \Phi(x)y'$ vanishes at the zeros of y hence there is a polynomial r of degree (at most) $N - 2$ such that (1.5) holds. This shows that the number of different solutions to (1.6) is the same as the number of choices of the polynomial r in (1.5). It is exactly this set up that is behind the modern Bethe Ansatz equations where second order differential equations are replaced by second order equations in the Askey-Wilson operator (XXZ model) or the Wilson operator (XXX model).

The paper is organized as follows. In Section 2, we indicate the equivalence of (1.6) to second order equations in the Askey-Wilson operator, which is a system of equations that generalize the Bethe Ansatz equations for the XXZ model. In Section 3 we provide intuitive explanations for closed form polynomial solutions to second order differential equations with polynomial coefficients of degrees 2, 1, and zero, as well as similar equations where derivatives are replaced by applications of q -difference and Askey-Wilson operators. This explains where the big q -Jacobi polynomials and the Askey-Wilson polynomials come from.

Section 4 is devoted to studying the general second order equation in the Askey-Wilson operator \mathcal{D}_q with general polynomial coefficients. We identify the symmetric form of such operator equation through an amazing simplification resulting from expanding the coefficients in Chebyshev polynomials of the first and second kinds. These representations lead in Section 5 to the concept of regular singular points of the second order operator equation in an Askey-Wilson operator with polynomial coefficients.

In Section 6, we consider the case corresponding to $q = 1$ in Section 4. The relationship of the Sturm-Liouville problem in terms of Wilson operator and the Bethe Ansatz equations of the XXX model for the ground state has been found.

Convention. In this paper, $\mathbf{Z}, \mathbf{R}, \mathbf{C}$ will denote the ring of integers, real, complex numbers respectively, $\mathbf{N} = \mathbf{Z}_{>0}$, $\mathbf{R}^* = \mathbf{R} \setminus \{0\}$, $\mathbf{C}^* = \mathbf{C} \setminus \{0\}$, and $i = \sqrt{-1}$.

2 q -Sturm-Liouville Problems

Given a function f , we set $\check{f}(z) = f(x)$ with

$$z = e^{i\theta}, \quad x = \cos \theta = (z + z^{-1})/2.$$

Indeed $z = x \pm \sqrt{x^2 - 1}$ with the branch of the square root chosen to make $\sqrt{x^2 - 1} \approx x$, as $x \rightarrow \infty$. This makes $|z^{-1}| \leq 1 \leq |z|$, and $=$ holds if and only if $x \in [-1, 1]$. With this notation

we now introduce the following operations on $f(x)$,

$$\begin{aligned}(\eta_q f)(x) &= \check{f}(q^{1/2}z), \\(\mathcal{D}_q f)(x) &= \frac{(1-x^2)^{-1/2}}{i(q^{1/2}-q^{-1/2})}(\eta_q f - \eta_{q^{-1}} f)(x), \\(\mathcal{A}_q f)(x) &= \frac{1}{2}(\eta_q f + \eta_{q^{-1}} f)(x).\end{aligned}\tag{2.1}$$

The operator \mathcal{D}_q is called the Askey-Wilson operator [9], [12]. It is important to observe that both \mathcal{D}_q and \mathcal{A}_q are invariant under $q \rightarrow q^{-1}$.

Recall that the Chebyshev polynomials of the first and second kinds, respectively, are

$$T_n(\cos \theta) = \cos n\theta, \quad U_n(\cos \theta) = \frac{\sin(n+1)\theta}{\sin \theta}.\tag{2.2}$$

The Askey-Wilson operator has the properties

$$\mathcal{D}_q T_n(x) = \frac{q^{n/2} - q^{-n/2}}{q^{1/2} - q^{-1/2}} U_{n-1}(x), \quad \mathcal{A}_q T_n(x) = \frac{1}{2} [q^{n/2} + q^{-n/2}] T_n(x).$$

Thus \mathcal{D}_q reduces the degree of a polynomial by 1 while \mathcal{A}_q preserves the degree of a polynomial. Furthermore the Askey-Wilson operator has the following properties, [12],

$$\begin{aligned}\mathcal{D}_q(fg) &= (\eta_q f)(\mathcal{D}_q g) + (\eta_{q^{-1}} g)(\mathcal{D}_q f) \\ &= (\mathcal{A}_q f)(\mathcal{D}_q g) + (\mathcal{A}_q g)(\mathcal{D}_q f).\end{aligned}\tag{2.3}$$

The second line in the above equation follows from the first by interchanging f and g in the first line then taking the average of the two answers.

Thus $\mathcal{D}_q, \mathcal{A}_q$ are operators of the polynomial algebra $\mathbf{C}[x]$ with $\deg \mathcal{D}_q(f) = \deg f - 1$, and $\deg \mathcal{A}_q(f) = \deg f$ for $f \in \mathbf{C}[x]$. Furthermore these operators preserve $\mathbf{R}[x]$ for a real q .

For convenience, we shall use the following convention throughout this paper,

$$q = e^{2i\eta}, \quad \theta = 2\lambda, \quad (\text{hence } x = \cos 2\lambda).\tag{2.4}$$

For given functions $w(x)$, $p(x)$, $r(x)$, we consider the following q -Sturm-Liouville equation of $f(x)$,

$$\frac{1}{w(x)} \mathcal{D}_q((p(x) \mathcal{D}_q f)(x)) = r(x) f(x).\tag{2.5}$$

By (2.3), one can rewrite the equation (2.5) in the following form,

$$\Pi(x) \mathcal{D}_q^2 f(x) + \Phi(x) (\mathcal{A}_q \mathcal{D}_q f)(x) = r(x) f(x),\tag{2.6}$$

where the functions Π, Φ are defined by

$$\Pi(x) = \frac{1}{w(x)} \mathcal{A}_q p(x), \quad \Phi(x) = \frac{1}{w(x)} \mathcal{D}_q p(x).\tag{2.7}$$

The form (2.5) is the symmetric form of (2.6), which can be seen from the formula of integration by parts in [7] which will be stated later as (5.3). We shall show in §4 how to construct w and p from Π and Φ . Now the relationship

$$\begin{aligned} (\mathcal{A}_q \mathcal{D}_q f)(x) &= \frac{q e^{i\theta}}{(q-1)(qe^{2i\theta}-1)(e^{2i\theta}-q)} \\ &\quad \times \{(e^{2i\theta}-q)\eta_{q^2} - (qe^{2i\theta}-1)\eta_{q^{-2}} + (q-1)(e^{2i\theta}+1)\} f(x); \\ \mathcal{D}_q^2 f(x) &= \frac{2q^{3/2} e^{i\theta}}{i(1-q)^2 \sin \theta (qe^{2i\theta}-1)(e^{2i\theta}-q)} \\ &\quad \times \{(e^{2i\theta}-q)\eta_{q^2} + (qe^{2i\theta}-1)\eta_{q^{-2}} - (q+1)(e^{2i\theta}-1)\} f(x), \end{aligned}$$

shows that a root $x_0 = \cos 2\lambda_0$ of the polynomial $f(x)$, $f(x_0) = 0$, necessarily satisfies the following equation,

$$\begin{aligned} &\{(e^{4i\lambda_0}-q)(\Pi(x_0)-\Phi(x_0)\sin \eta \sin 2\lambda_0)\eta_{q^2}\} f(x_0) \\ &+ \{(qe^{4i\lambda_0}-1)(\Pi(x_0)+\Phi(x_0)\sin \eta \sin 2\lambda_0)\eta_{q^{-2}}\} f(x_0) = 0, \end{aligned}$$

or equivalently,

$$\left(\frac{\eta_{q^2} f}{\eta_{q^{-2}} f} \right) (x_0) = \frac{-\sin(2\lambda_0 + \eta)(\Pi(x_0) + \Phi(x_0)\sin \eta \sin 2\lambda_0)}{\sin(2\lambda_0 - \eta)(\Pi(x_0) - \Phi(x_0)\sin \eta \sin 2\lambda_0)}. \quad (2.8)$$

For a polynomial $f(x)$ of degree n with distinct simple roots x_1, \dots, x_n , one writes

$$f(x) = \gamma \prod_{j=1}^n (x - x_j) = \gamma \prod_{j=1}^n (\cos 2\lambda - \cos 2\lambda_j), \quad \gamma \neq 0.$$

It is straight forward to see that

$$\begin{aligned} \eta_{q^2} f(x_k) &= \frac{\gamma}{2^n} \prod_{j=1}^n (qe^{2i\lambda_k} - e^{2i\lambda_j} + q^{-1}e^{-2i\lambda_k} - e^{-2i\lambda_j}), \\ &= \frac{\gamma}{2^n} \prod_{j=1}^n \left\{ e^{i(\eta+\lambda_k+\lambda_j)} (e^{i(\eta+\lambda_k-\lambda_j)} - e^{-i(\eta+\lambda_k-\lambda_j)}) - e^{-i(\eta+\lambda_k+\lambda_j)} (e^{i(\eta+\lambda_k-\lambda_j)} - e^{-i(\eta+\lambda_k-\lambda_j)}) \right\} \\ &= (-1)^n \gamma \prod_{j=1}^n \sin(\lambda_k + \lambda_j + \eta) \sin(\lambda_k - \lambda_j + \eta); \\ \eta_{q^{-2}} f(x_k) &= \frac{\gamma}{2^n} \prod_{j=1}^n (q^{-1}e^{2i\lambda_k} - e^{2i\lambda_j} + qe^{-2i\lambda_k} - e^{-2i\lambda_j}), \\ &= (-1)^n \gamma \prod_{j=1}^n \sin(\lambda_k + \lambda_j - \eta) \sin(\lambda_k - \lambda_j - \eta). \end{aligned}$$

Now observe that (2.8) indicates that the roots x_1, \dots, x_n of $f(x)$ satisfy the system of equations,

$$\begin{aligned} &\frac{-\sin(2\lambda_k + \eta)(\Pi(x_k) + \Phi(x_k)\sin \eta \sin 2\lambda_k)}{\sin(2\lambda_k - \eta)(\Pi(x_k) - \Phi(x_k)\sin \eta \sin 2\lambda_k)} \\ &= \prod_{j=1}^n \frac{\sin(\lambda_k + \lambda_j + \eta) \sin(\lambda_k - \lambda_j + \eta)}{\sin(\lambda_k + \lambda_j - \eta) \sin(\lambda_k - \lambda_j - \eta)}, \quad 1 \leq k \leq n. \end{aligned}$$

In other words we arrive at the system of nonlinear equations

$$\frac{\Pi(x_k) + \Phi(x_k) \sin \eta \sin 2\lambda_k}{\Pi(x_k) - \Phi(x_k) \sin \eta \sin 2\lambda_k} = \prod_{j \neq k, j=1}^n \frac{\sin(\lambda_k + \lambda_j + \eta) \sin(\lambda_k - \lambda_j + \eta)}{\sin(\lambda_k + \lambda_j - \eta) \sin(\lambda_k - \lambda_j - \eta)}, \quad 1 \leq k \leq n, \quad (2.9)$$

which we call the Bethe Ansatz equations associated with $\Pi(x), \Phi(x)$. For the interest of applications to physical problems, we shall only consider those q -Sturm-Liouville problem where the coefficients $\Pi(x), \Phi(x), r(x)$ of (2.6) are polynomials in x with the degrees

$$\deg \Pi = 1 + \deg \Phi = 2 + \deg r = N \geq 2. \quad (2.10)$$

3 Second Order Equations

We first introduce some notations from [2], [9]. The q -shifted factorials are defined by

$$(a; q)_0 = 1, \quad (a; q)_n = \prod_{k=1}^n (1 - aq^{k-1}), \quad n = 1, \dots, \text{ or } \infty. \quad (3.1)$$

Furthermore

$$(a; q)_\alpha := \frac{(a; q)_\infty}{(aq^\alpha; q)_\infty}. \quad (3.2)$$

Formula (3.2) clearly holds when α is a nonnegative integer but is used to define the general q -shifted factorial when α is not necessarily an integer.

Askey and Wilson [4] introduced the polynomials,

$$\phi_n(\cos \theta; a) := (ae^{i\theta}, ae^{-i\theta}; q)_n \equiv (ae^{i\theta}; q)_n (ae^{-i\theta}; q)_n, \quad (3.3)$$

as a basis for the space of polynomials. This is the most suitable basis for use here. A different basis appeared in the q -exponential functions in [15] where it was used to provide a q -analogue of the expansion of a plane wave in spherical harmonics. Clearly

$$\phi_n(x; a) = (-2a)^n q^{n(n-1)/2} x^n + \text{lower order terms}. \quad (3.4)$$

It is straightforward to see that

$$\lim_{q \rightarrow 1} \phi_n(x; a) = (1 - ae^{i\theta})^n (1 - ae^{-i\theta})^n = (1 - 2ax + a^2)^n.$$

We may use (3.2) to define the more general functions $\{\phi_\alpha(x; a)\}$ by (3.3) when α is not necessarily an integer. It readily follows that

$$\begin{aligned} \mathcal{D}_q \phi_\alpha(x; a) &= \frac{(1-q^\alpha)}{2a(q-1)} \phi_{\alpha-1}(x; aq^{1/2}), \\ \mathcal{A}_q \phi_\alpha(x; a) &= \phi_{\alpha-1}(x; aq^{1/2}) [1 - aq^{-1/2}(1 + q^\alpha)x + a^2 q^{\alpha-1}]. \end{aligned} \quad (3.5)$$

The second formula in (3.5) holds when $\alpha = 0$ provided that we interpret the product defining ϕ_α in (3.3) as in (3.2). Furthermore we have

$$2\mathcal{A}_q \phi_\alpha(x; a) = (1 + q^{-\alpha}) \phi_\alpha(x; aq^{1/2}) + (1 - q^{-\alpha})(1 + a^2 q^{2\alpha-1}) \phi_{\alpha-1}(x; aq^{1/2}). \quad (3.6)$$

We shall use $\pi_j(x)$ to denote a generic polynomial in x of degree j . Consider a differential equation

$$\pi_2(x)y''(x) + \pi_1(x)y'(x) + \lambda y(x) = 0, \quad (3.7)$$

where λ is a constant. We seek a polynomial solution to (3.7) of degree n . We know that one of the coefficients in π_1 or π_2 is not zero, hence there is no loss of generality in choosing it equal to 1. Thus π_1 and π_2 contain four free parameters. The scaling $x \rightarrow ax + b$ of the independent variable absorbs two of the four parameters. The eigenvalue parameter λ is then uniquely determined by equating coefficients of x^n in (3.7) since y has degree n . This reduces (3.7), in general, to a Jacobi differential equation whose polynomial solution, in general, is a Jacobi polynomial, see [22]. Solutions also include special and limiting cases of Jacobi polynomials including the Bessel polynomials and the polynomial x^n .

Next let us consider the same problem for the operator

$$(D_q f)(x) = \frac{f(x) - f(qx)}{x - qx}. \quad (3.8)$$

Consider the operator equation

$$\pi_2(x)D_q^2 y(x) + \pi_1(x)D_q y(x) + \lambda y(x) = 0. \quad (3.9)$$

Here under the same assumptions on π_1 and π_2 one easily finds out that the only scaling allowed on x is $x \rightarrow ax$, hence one of the coefficients in π_1 and π_2 is chosen as 1 and the remaining coefficients of π_1 and π_2 constitute three free parameters. The general polynomial solution to (3.9) is the big q -Jacobi polynomial which contains three free parameters, [16], [9], [2].

We next consider the Askey-Wilson case

$$\pi_2(x)\mathcal{D}_q^2 y(x) + \pi_1(x)\mathcal{A}_q \mathcal{D}_q y(x) + \lambda y(x) = 0. \quad (3.10)$$

In this case one can not perform any scaling on x , so apart from assuming that one of the coefficients in π_1 and π_2 is unity, we have four free parameter, namely the remaining coefficients in π_2 and the coefficients in π_1 . This is the case of the Askey-Wilson polynomials where

$$\begin{aligned} \pi_2(x) &= -q^{-1/2} [2(1 + \sigma_4)x^2 - (\sigma_1 + \sigma_3)x - 1 + \sigma_2 - \sigma_4], \\ \pi_1(x) &= 2[2(\sigma_4 - 1)x + \sigma_1 - \sigma_3] / (1 - q), \end{aligned} \quad (3.11)$$

where σ_j is the j th elementary symmetric function of parameters a_1, a_2, a_3, a_4 . In order to solve (3.10) for y we expand y in the Askey-Wilson basis $\{\phi_n(x; a_1)\}$ and find

$$\lambda = -4q(1 - q^{-n})(1 - \sigma_4 q^{n-1})(1 - q)^{-2}. \quad (3.12)$$

With the above choice for λ the polynomial solution to (3.3) is unique and is given by an Askey-Wilson polynomial of degree n , see for example [7].

At this stage one wonders whether replacing π_2, π_1 and λ by π_{k+1}, π_k , and π_{k-1} in equations (3.7), (3.9) and (3.10) lead to more general orthogonal polynomials. Grunbaum and Haine

[10] proved that the only orthogonal polynomial solutions to (3.10) after the replacements $(\pi_2, \pi_1, \lambda) \rightarrow (\pi_{k+1}, \pi_k, \pi_{k-1})$ are the Askey-Wilson polynomials or special and limiting cases of them. Ismail [13] showed that the same conclusion holds without assuming orthogonality. This generalizes earlier work of Hahn, and Bochner who proved that the q -Jacobi polynomials, and the Jacobi polynomials are the only polynomial solutions to (3.9) and (3.7), respectively with the above replacements.

4 Multiparameter Cases and Bethe Ansatz Equations for the XXZ Model

For $2N$ complex numbers $a_j, 1 \leq j \leq 2N$, we denote

$$\vec{a} = (a_1, \dots, a_{2N}),$$

and σ_j the j -th elementary symmetric function of a_i 's for $0 \leq j \leq 2N$, with $\sigma_0 := 1$. We define the weight function $w(x, \vec{a})$,

$$w(x, \vec{a}) := \frac{(e^{iN\theta}, e^{-iN\theta}; q^{\frac{N}{2}})_\infty}{\sin \frac{N\theta}{2} \prod_{j=1}^{2N} (a_j e^{i\theta}, a_j e^{-i\theta}; q)_\infty}, \quad (4.1)$$

which can also be written in the following form,

$$w(x, \vec{a}) = \frac{2ie^{-\frac{iN\theta}{2}} (e^{iN\theta}, q^{\frac{N}{2}} e^{-iN\theta}; q^{\frac{N}{2}})_\infty}{\prod_{j=1}^{2N} (a_j e^{i\theta}, a_j e^{-i\theta}; q)_\infty} = \frac{-2ie^{\frac{iN\theta}{2}} (q^{\frac{N}{2}} e^{iN\theta}, e^{-iN\theta}; q^{\frac{N}{2}})_\infty}{\prod_{j=1}^{2N} (a_j e^{i\theta}, a_j e^{-i\theta}; q)_\infty}. \quad (4.2)$$

With $w(x) = w(x, \vec{a})$, $p(x) = w(x, q^{1/2} \vec{a})$ in (2.5), we shall consider the following equations,

$$\frac{1}{w(x, \vec{a})} \mathcal{D}_q((w(x, q^{1/2} \vec{a}) \mathcal{D}_q y)(x)) = r(x)y(x), \quad r(x) \in \mathbf{C}[x], \quad \deg r = N - 2. \quad (4.3)$$

With the notation

$$\Pi(x; \vec{a}) = \frac{1}{w(x, \vec{a})} \mathcal{A}_q w(x, q^{1/2} \vec{a}), \quad \Phi(x; \vec{a}) = \frac{1}{w(x, \vec{a})} \mathcal{D}_q w(x, q^{1/2} \vec{a}), \quad (4.4)$$

the equation in (4.3) becomes

$$\Pi(z; \vec{a}) \mathcal{D}_q^2 y + \Phi(z; \vec{a}) \mathcal{A}_q \mathcal{D}_q y = r(x)y. \quad (4.5)$$

Note that for $N = 2$, $r(x) = r \in \mathbf{R}$ and $a_j, q \in \mathbf{R}$ with $|a_j| < 1, 0 < q < 1$, the weight function $w_{\vec{a}}(x)$ is a positive function on $(-1, 1)$, and the solutions of the equation (4.3) are the Askey-Wilson polynomials which are orthogonal in $L^2((-1, 1); (1 - x^2)^{-1/2})$, see e.g. [7].

Theorem 4.1 *The functions $\Pi(x; \vec{a}), \Phi(x; \vec{a})$ are polynomials of x of degree $N, N - 1$ respectively, and have the following explicit forms,*

$$\Pi(x; \vec{a}) = -q^{-N/4} \{(-1)^N \sigma_N + \sum_{l=0}^{N-1} (-1)^l (\sigma_l + \sigma_{2N-l}) T_{N-l}(x)\}, \quad (4.6)$$

$$\Phi(x; \vec{a}) = \frac{2q^{-N/4}}{q^{1/2} - q^{-1/2}} \sum_{l=0}^{N-1} (-1)^l (\sigma_l - \sigma_{2N-l}) U_{N-l-1}(x). \quad (4.7)$$

Conversely, for given polynomials Π and Φ of degrees N and $N - 1$ respectively, there is a unique $2N$ -element set $\{a_j : 1 \leq j \leq 2N\}$ such that $\Pi(x) = \Pi(x, \vec{a})$ and $\Phi(x) = \Phi(x; \vec{a})$ and (4.4) holds.

Proof: By the definition of $w(x, \vec{a})$, also the forms in (4.2) when applying $\eta_q, \eta_{q^{-1}}, \Pi(x; \vec{a})$ has the following expression,

$$\frac{iq^{\frac{-N}{4}} \sin \frac{N\theta}{2} \prod_{j=1}^{2N} (a_j e^{i\theta}, a_j e^{-i\theta}; q)_\infty}{(e^{iN\theta}, e^{-iN\theta}; q^{\frac{N}{2}})_\infty} \left[\frac{e^{\frac{-iN\theta}{2}} (q^{\frac{N}{2}} e^{iN\theta}, e^{-iN\theta}; q^{\frac{N}{2}})_\infty}{\prod_{j=1}^{2N} (a_j q e^{i\theta}, a_j e^{-i\theta}; q)_\infty} - \frac{e^{\frac{iN\theta}{2}} (e^{iN\theta}, q^{\frac{N}{2}} e^{-iN\theta}; q^{\frac{N}{2}})_\infty}{\prod_{j=1}^{2N} (a_j e^{i\theta}, a_j q e^{-i\theta}; q)_\infty} \right],$$

which implies

$$\begin{aligned} \Pi(x; \vec{a}) &= iq^{\frac{-N}{4}} \sin \frac{N\theta}{2} \left[\frac{e^{\frac{-iN\theta}{2}}}{1 - e^{iN\theta}} \prod_{j=1}^{2N} (1 - a_j e^{i\theta}) - \frac{e^{\frac{iN\theta}{2}}}{1 - e^{-iN\theta}} \prod_{j=1}^{2N} (1 - a_j e^{-i\theta}) \right] \\ &= \frac{-q^{\frac{-N}{4}}}{2} \left[e^{-iN\theta} \prod_{j=1}^{2N} (1 - a_j e^{i\theta}) + e^{iN\theta} \prod_{j=1}^{2N} (1 - a_j e^{-i\theta}) \right] \\ &= \frac{-q^{\frac{-N}{4}}}{2} \sum_{l=0}^{2N} (-1)^l \sigma_l (e^{i(l-N)\theta} + e^{i(N-l)\theta}) = -q^{\frac{-N}{4}} \sum_{l=0}^{2N} (-1)^l \sigma_l \cos(N-l)\theta \\ &= -q^{\frac{-N}{4}} \{ (-1)^N \sigma_N + \sum_{l=0}^{N-1} (-1)^l (\sigma_l + \sigma_{2N-l}) T_{N-l}(x) \}. \end{aligned}$$

By the same method, we have

$$\begin{aligned} \Phi(x; \vec{a}) &= \frac{2q^{\frac{-N}{4}} \sin \frac{N\theta}{2}}{(q^{1/2} - q^{-1/2}) \sin \theta} \left[\frac{e^{\frac{-iN\theta}{2}}}{1 - e^{iN\theta}} \prod_{j=1}^{2N} (1 - a_j e^{i\theta}) + \frac{e^{\frac{iN\theta}{2}}}{1 - e^{-iN\theta}} \prod_{j=1}^{2N} (1 - a_j e^{-i\theta}) \right] \\ &= \frac{iq^{\frac{-N}{4}}}{(q^{1/2} - q^{-1/2}) \sin \theta} \left[e^{-iN\theta} \prod_{j=1}^{2N} (1 - a_j e^{i\theta}) - e^{iN\theta} \prod_{j=1}^{2N} (1 - a_j e^{-i\theta}) \right] \quad (4.8) \\ &= \frac{iq^{\frac{-N}{4}}}{(q^{1/2} - q^{-1/2}) \sin \theta} \sum_{l=0}^{2N} (-1)^l \sigma_l (e^{i(l-N)\theta} - e^{i(N-l)\theta}) \\ &= \frac{2q^{\frac{-N}{4}}}{(q^{1/2} - q^{-1/2})} \sum_{l=0}^{2N} (-1)^l \sigma_l \frac{\sin(N-l)\theta}{\sin \theta} \\ &= \frac{2q^{\frac{-N}{4}}}{(q^{1/2} - q^{-1/2})} \sum_{l=0}^{N-1} (-1)^l (\sigma_l - \sigma_{2N-l}) U_{N-l-1}(x). \end{aligned}$$

To see the converse statement, given Π and Φ we expand them in Chebyshev polynomials of the first and second kinds respectively, then define σ_0 by $\sigma_0 = 1$ and σ_N by $(-1)^{N+1} q^{N/4}$ times the constant term in the expansion (4.6) in terms of Chebyshev polynomials. Then define the remaining σ 's through finding $\sigma_l \pm \sigma_{2N-l}$ from the coefficients in Π and Φ in (4.6) and (4.7). \square

It is important to note that Theorem 4.1 gives a constructive way of identifying the parameters a_1, \dots, a_{2N} and $w(x; \vec{a})$ from the functional equation (4.5).

Theorem 4.2 Let $a_l = q^{-s_l} = e^{-2i\eta s_l}$ for $1 \leq l \leq 2N$. The Bethe Ansatz equations (2.9) associated with the polynomials $\Pi(x; \vec{a}), \Phi(x; \vec{a})$ have the form (1.3).

Proof: By Theorem 4.1, (indeed in its proof), we have

$$\begin{aligned}\Pi(x; \vec{a}) &= \frac{-q^{\frac{-N}{4}}}{2} \left[e^{-2iN\lambda_k} \prod_{j=1}^{2N} (1 - a_j e^{2i\lambda_k}) + e^{2iN\lambda_k} \prod_{j=1}^{2N} (1 - a_j e^{-2i\lambda_k}) \right] \\ \Phi(x_k; \vec{a}) \sin \eta \sin 2\lambda_k &= \frac{q^{\frac{-N}{4}}}{2} \left[e^{-2iN\lambda_k} \prod_{j=1}^{2N} (1 - a_j e^{2i\lambda_k}) - e^{2iN\lambda_k} \prod_{j=1}^{2N} (1 - a_j e^{-2i\lambda_k}) \right],\end{aligned}$$

hence

$$\begin{aligned}\Pi(x_k; \vec{a}) + \Phi(x_k; \vec{a}) \sin \eta \sin 2\lambda_k &= -q^{\frac{-N}{4}} e^{2iN\lambda_k} \prod_{j=1}^{2N} (1 - a_j e^{-2i\lambda_k}) \\ &= -q^{\frac{-N}{4}} e^{-2iN\lambda_k} \prod_{j=1}^{2N} (e^{2i\lambda_k} - a_j), \\ \Pi(x_k; \vec{a}) - \Phi(x_k; \vec{a}) \sin \eta \sin 2\lambda_k &= -q^{\frac{-N}{4}} e^{-2iN\lambda_k} \prod_{j=1}^{2N} (1 - a_j e^{2i\lambda_k}).\end{aligned}$$

By substituting $a_j = q^{-s_j}$ in the above formula, the result of this theorem follows from (2.9).

□

If $|q| > 1$ replace q by $1/p$, use the invariance of \mathcal{D}_q and \mathcal{A}_q under $q \rightarrow q^{-1}$ to rederive Theorem 4.2 with q replaced by $1/p$. This covers the case $|q| > 1$. The cases $|q| = 1$ and in particular the cases when q is a root of unity do not seem to be amenable to the techniques developed here.

The Bethe Ansatz equations (2.9) describe the relations of roots $x_j, 1 \leq j \leq n$, of a polynomial $f(x)$ of degree n in the q -Sturm-Liouville problem (4.3). It is important to note that for given Π and Φ in (2.6) with $\deg \Pi = N$ and $\deg \Phi = N - 1$, there are $2N$ complex numbers, a_1, a_2, \dots, a_{2N} , such that $\Pi(x) = \Pi(x; \vec{a})$ and $\Phi(x) = \Phi(x; \vec{a})$. For a positive integer N and all $a_j = q^{-s}$ with $s \in \frac{1}{2}\mathbf{Z}_{\geq 0}$, the equation (2.9), or (1.3) become (1.2) which is the Bethe Ansatz equations for the spin s XXZ model of a size $2N$ with the open (Dirichlet) boundary condition [21]. This correspondence shows that identifying the spectrum of XXZ spin chain is related to spectral problems of a q -Sturm-Liouville equation.

For $N = 2$, we have $\Pi(x; \vec{a}) = \pi_2(x)$ and $\Phi(x; \vec{a}) = \pi_1(x)$ in (3.11). In the special case

$$a_1 = -a_2 = e^{-is}, \quad a_3 = -a_4 = e^{-i(s+\eta)},$$

the polynomial solution to (4.3) is a q -ultraspherical polynomial of degree n . In this case (1.3) becomes

$$\frac{\sin(2\lambda_k + s) \sin(2\lambda_k + s + \eta)}{\sin(2\lambda_k - s) \sin(2\lambda_k - s - \eta)} = \prod_{j \neq k, j=1}^n \frac{\sin(\lambda_k + \lambda_j - \eta) \sin(\lambda_k - \lambda_j - \eta)}{\sin(\lambda_k + \lambda_j + \eta) \sin(\lambda_k - \lambda_j + \eta)}, \quad 1 \leq k \leq n.$$

For $N = 2$ with $s_j < 0$ for all j , $y(x)$ is an Askey-Wilson polynomial of degree n . In fact, one has the following result.

Theorem 4.3 *Let $N = 2$ and $\eta = i\zeta$, $\zeta > 0$. Then for all n the system (1.3) has a unique solution provided that $s_j < 0$, $1 \leq j \leq 4$. Furthermore all the λ 's are in $(0, \pi/2)$.*

Proof. Let y be a polynomial of degree n with zeros $\cos(2\lambda_j)$, $1 \leq j \leq n$. We know that (1.3) implies the validity of (3.10) for $x = \cos(2\lambda_j)$. Here π_1 and π_2 are as in (3.10). With λ in (3.9) chosen as in (3.12) the left-hand side of (3.10) is a polynomial in x of degree $n - 1$ and vanishes at n points. Hence (3.10) must hold for all x , and y must be an Askey-Wilson polynomial of degree n . Since the Askey-Wilson polynomials are orthogonal on $[-1, 1]$, all their zeros are in $(-1, 1)$. \square

For large n the distribution of the $\cos(2\lambda_j)$'s follows is an arcsine distribution. This follows from general theory of orthogonal polynomials since in this case $\int_{-1}^1 \ln w(x)(1 - x^2)^{-1/2} dx$ is finite [19], [20]. Note that the proof of Theorem 4.3 used the orthogonality of the Askey-Wilson polynomials in an essential way.

Using arguments that go back to Heine, one can prove that for given polynomials Π and Φ of degree N and $N - 1$ respectively, there exist at most $\binom{N+n-2}{N-2}$ choices of $r(x)$ such that (2.6) has a polynomial solution of degree n . This shows that for $N > 2$ the solution to (1.3), without additional assumptions, may not be unique.

For $a_j = q^{-s_j}$ the monic Askey-Wilson polynomials satisfy the recurrence relation

$$xp_n(x) = p_{n+1}(x) + (\cos 2\eta + 2A_n + 2C_n)p_n(x) + 4A_{n-1}C_n p_{n-1}(x), \quad (4.9)$$

where

$$\begin{aligned} A_n &= \frac{\sin((n-1-\sigma'_1)\eta) \prod_{j=2}^4 \sin((n-s_1-s_j)\eta)}{\sin((2n-1-\sigma'_1)\eta) \sin((2n-\sigma'_1)\eta)}, \\ C_n &= \frac{\sin(n\eta) \prod_{2 \leq j < k \leq 4} \sin((n-1-s_j-s_k)\eta)}{\sin((2n-1-\sigma'_1)\eta) \sin((2n-2-\sigma'_1)\eta)}, \end{aligned} \quad (4.10)$$

and σ'_j is the j th elementary symmetric function of the s_k 's, (see (3.1.4)-(3.1.5) in [16]). From the form of A_n and C_n in (4.10) it is clear that the positivity condition $A_{n-1}C_n > 0$ may not hold for all n .

Theorem 4.4 *Assume that η and all the s_j 's are real and that $A_0C_1 > 0$. Let*

$$M = \text{Max}\{n : A_{k-1}C_k > 0, \text{ for } 1 \leq k \leq n\}.$$

Then (1.3) has a unique solution for $0 \leq n \leq M$ and the λ 's are all real and simple.

Proof. We have a family of $M + 1$ (which may be $= \infty$) orthogonal polynomials and their zeros are all real and simple. It is known that in this case (4.5) has only one polynomial solution [5].

\square

Remark: It is important to emphasize that when the orthogonality condition $A_{n-1}C_n > 0$ is violated, then the Askey-Wilson polynomials continue to satisfy (4.5), hence their zeros solve the Bethe Ansatz equations but we can no longer guarantee the reality or the simplicity of the zeros of the Askey-Wilson polynomials. \square

5 Singularities and Expansions

In this section we consider different regimes. We assume $0 < q < 1$ so $\imath\eta < 0$ only in (5.1)-(5.4) below. Recall the inner product associated with the Chebyshev weight $(1-x^2)^{-1/2}$ on $(-1, 1)$, namely

$$\langle f, g \rangle := \int_{-1}^1 f(x) \overline{g(x)} \frac{dx}{\sqrt{1-x^2}}. \quad (5.1)$$

For $0 < q < 1$, one observes that the definition (2.1) requires $\check{f}(z)$ to be defined for $|q^{\pm 1/2}z| = 1$ as well as for $|z| = 1$. In particular \mathcal{D}_q is well-defined on $H_{1/2}$, where

$$H_\nu := \{f : f((z + 1/z)/2) \text{ is analytic for } q^\nu \leq |z| \leq q^{-\nu}\}. \quad (5.2)$$

Brown, Evans, and Ismail [7] proved the integration by parts formula

$$\begin{aligned} \langle \mathcal{D}_q f, g \rangle &= \frac{\pi \sqrt{q}}{1-q} \left[f\left(\frac{1}{2}(q^{1/2} + q^{-1/2})\right) \overline{g(1)} - f\left(-\frac{1}{2}(q^{1/2} + q^{-1/2})\right) \overline{g(-1)} \right] \\ &\quad - \langle f, \sqrt{1-x^2} \mathcal{D}_q(g(x) (1-x^2)^{-1/2}) \rangle, \end{aligned} \quad (5.3)$$

for $f, g \in H_{1/2}$. They also proved that if $w(x) > 0$ on $(-1, 1)$, and $y \in H_1$, $p \in H_1$ then the eigenvalues of the q -Sturm-Liouville problem,

$$\frac{1}{w(x)} \mathcal{D}_q(p(x) \mathcal{D}_q y(x)) = \lambda y(x), \quad (5.4)$$

are real and the eigenfunctions corresponding to distinct eigenvalues are orthogonal with respect to w . This implies the following theorem.

Theorem 5.1 *Assume that $0 < q < 1$, $|a_j| < q^{1/2}$, $1 \leq j \leq 4$, and $w(x; \vec{a}) > 0$ on $(-1, 1)$ where $\vec{a} = (a_1, a_2, a_2, a_4)$. Then the eigenvalues of*

$$\frac{1}{w(x, \vec{a})} \mathcal{D}_q \left(w(x, q^{1/2} \vec{a}) \mathcal{D}_q y(x) \right) = \lambda y(x),$$

are real and simple, and the eigenfunctions are mutually orthogonal on $(-1, 1)$ with respect to the weight function $w(x; \vec{a})$.

Proof. The condition $|a_j| < q^{1/2}$, $1 \leq j \leq 4$ ensures that $p(x) = w(x; q^{1/2} \vec{a})$ is in H_1 and the theorem follows from [7]. \square

We now discuss the concept of a regular singular point of the equation (4.3), which is the general form of a second order equation in the Askey-Wilson operator with polynomial coefficients as we say in Theorem 4.1 for a general q and N .

First recall that the concept of singularities of differential equations is related to the analytic properties of the solutions in a neighborhood of the singularities. We have no geometric way to describe the corresponding situation for equations like (4.3). In the present set up the analogue of a function analytic in a neighborhood of a point $(a + a^{-1})/2$ is a function which has a convergent series expansion of the form $\sum_{n=0}^{\infty} c_n \phi_n(x; a)$. We have no other characterization of these q -analytic functions.

In the case of second order differential equations the singularities are the zeros of the coefficient of y'' and the regular singular points ζ_j 's are precisely those points where one can construct a series solution to the differential equation of the form $\sum_{n=0}^{\infty} c_n (z - \zeta_j)^{\alpha_j + n}$ in a neighborhood of $z = \zeta_j$. A closer examination of the equation (4.3) in the form (4.5) reveals that one can formally expand a solution y as $\sum_{n=0}^{\infty} y_n \phi_n(x; a)$, substitute the series expansion in (4.5) and recursively compute the coefficients y_n provided that a is not among the $2N$ parameters $\{\zeta_1, \dots, \zeta_{2N}\}$, where $\zeta_j = (a_j + a_j^{-1})/2$, and possibly the points 0 and ∞ , which we do not know how to handle. This indicates that what plays the role of singular points of (4.5) are $\zeta_1, \dots, \zeta_{2N}$ in addition to $x = 0, x = \infty$. Around the singular point $x = \zeta_j$, we shall expand functions in the set $\{\phi_{n+\alpha}(x; a_j)\}$, where $\phi_{\alpha}(x; a)$ is as in (3.3). We let

$$y(x) = \sum_{n=0}^{\infty} y_n \phi_{n+\alpha}(x; a_1), \quad (5.5)$$

and observe that $r(x)\phi_{n+\alpha}(x; a_1)$ is a linear combination of $\{\phi_{m+\alpha}(x; a_1) : n \leq m \leq n+N-2\}$. Furthermore we note that (3.2), (3.3), and (4.4) imply

$$\begin{aligned} & \frac{1}{w(x; \vec{a})} \mathcal{D}_q \left(w(x; q^{1/2} \vec{a}) \mathcal{D}_q \phi_{n+\alpha}(x; a_1) \right) \\ &= \frac{1 - q^{n+\alpha}}{2a_1(q-1)w(x; \vec{a})} \mathcal{D}_q \left(w(x; q^{1/2} \vec{a}) \phi_{n+\alpha-1}(x; q^{1/2} a_1) \right) \\ &= \frac{1 - q^{n+\alpha}}{2a_1(q-1)w(x; \vec{a})} \mathcal{D}_q \left(w(x; a_1 q^{n+\alpha-1/2}, a_2, \dots, a_{2N}) \right) \\ &= \frac{(1 - q^{n+\alpha})w(x; a_1 q^{n+\alpha-1}, a_2, \dots, a_{2N})}{2a_1(q-1)w(x; \vec{a})} \Phi(x; a_1 q^{n+\alpha-1}, a_2, \dots, a_{2N}) \\ &= \frac{1 - q^{n+\alpha}}{2a_1(q-1)} \Phi(x; a_1 q^{n+\alpha-1}, a_2, \dots, a_{2N}) \phi_{n+\alpha-1}(x; a_1). \end{aligned}$$

The substitution of the expansion (5.5) for y in (4.3), reduces the left-hand side of (4.3) to

$$\sum_{n=0}^{\infty} \frac{1 - q^{n+\alpha}}{2a_1(q-1)} \Phi(x; a_1 q^{n+\alpha-1}, a_2, \dots, a_{2N}) \phi_{n+\alpha-1}(x; a_1) y_n. \quad (5.6)$$

Note that the smallest subscript of a ϕ in $r(x)y(x)$ in (4.5) is α . On the other hand (5.6) implies that $\phi_{\alpha-1}$ appears on the left-hand side of (4.3). Thus the coefficient of $\phi_{\alpha-1}(x; a_1)$ must be zero. To determine this coefficient we set

$$\Phi(x; q^{\alpha-1} a_1, a_2, \dots, a_{2N}) = \sum_{j=0}^{N-1} d_j (q^{\alpha}) \phi_j(x; a_1 q^{\alpha-1}), \quad (5.7)$$

and after making use of $\phi_n((a + a^{-1})/2; a) = \delta_{n,0}$ we find

$$d_0(q^\alpha) = \Phi((a_1 q^{\alpha-1} + a_1^{-1} q^{1-\alpha})/2; q^{\alpha-1} a_1, a_2, \dots, a_{2N}).$$

Thus the vanishing of the coefficient of $\phi_{\alpha-1}(x; a_1)$ on the left-hand side of (4.3) implies the vanishing of $(1 - q^\alpha)d_0(q^\alpha)$, that is

$$(1 - q^\alpha)\Phi((a_1 q^{\alpha-1} + a_1^{-1} q^{1-\alpha})/2; q^{\alpha-1} a_1, a_2, \dots, a_{2N}) = 0. \quad (5.8)$$

Theorem 5.2 *Assume $|a_j| \leq 1$, for all j . Then the only solution(s) of (5.8) are given by $q^\alpha = 1$, or $q^\alpha = q/(a_1 a_j)$, $j = 2, \dots, 2N$.*

Proof. From (5.8) it is clear that $q^\alpha = 1$ is a solution. With $x = (a_1 q^{\alpha-1} + a_1^{-1} q^{1-\alpha})/2$ as in (5.8) we find $e^{i\theta} = a_1 q^{\alpha-1}$, or $a_1^{-1} q^{1-\alpha}$. In the former case, $2i \sin \theta = a_1 q^{\alpha-1} - a_1^{-1} q^{1-\alpha}$, hence (5.8) and (4.8) imply

$$\frac{2i(1 - a_1^2 q^{2\alpha-2})}{a_1 q^{\alpha-1} - q^{1-\alpha}/a_1} \prod_{j=2}^{2N} (1 - a_1 a_j q^{\alpha-1}) = 0,$$

which gives the result. On the other hand if $e^{i\theta} = q^{1-\alpha}/a_1$, then we reach the same solutions via (4.8). \square

Ismail and Stanton [14] used two bases in addition to $\{\phi_n(x; a)\}$ for polynomial expansions. Their bases are

$$\rho_n(\cos \theta) := (1 + e^{2i\theta})(-q^{2-n} e^{2i\theta}; q^2)_{n-1} e^{-in\theta}, \quad (5.9)$$

$$\phi_n(\cos \theta) := (q^{1/4} e^{i\theta}, q^{1/4} e^{-i\theta}; q^{1/2})_n. \quad (5.10)$$

They satisfy

$$\mathcal{D}_q \rho_n(x) = 2q^{(1-n)/2} \frac{1 - q^n}{1 - q} \rho_{n-1}(x), \quad (5.11)$$

$$\mathcal{D}_q \phi_n(x) = -2q^{1/4} \frac{1 - q^n}{1 - q} \phi_{n-1}(x) \quad (5.12)$$

One can also seek solutions of second order operator equations by expanding solutions in the above polynomial basis. This will be the subject of future work.

Atakishiyev and Suslov [5] studied certain expansions of solutions of a very special non-homogenous equation corresponding to (3.10), that is $N = 2$, with special value of λ . They did not however investigate any concept of singularities, nor they have observed the general structure of expanding the polynomial coefficients in Chebyshev polynomials. Their Wronskian is inadequate because according to their definition, the Wronskian of two polynomials is not a polynomial. Askey and Wilson wrote down the functional equation (3.10) and identified it as the equation satisfied by the Askey-Wilson polynomials. Of course when one works only with the case $N = 2$, as in [5], one is bound to miss the complications and the elegance of the case of general N .

6 Bethe Ansatz Equations for the XXX Model and Wilson Operators

In this section we consider the problems arisen from the discussion in the previous sections when q tends to one, the corresponding Sturm-Liouville problem connecting with the Bethe Ansatz equations of the Heisenberg XXX spin chain. We write the variable z in previous sections in the form,

$$z = e^{i\theta} = q^{-iy},$$

and again the parameters, $a_j = q^{-sj}$. It is known that as q tends to 1, the transformation $\check{f}(z)$ and the operators $\eta_{q^{\pm 1}}, \mathcal{D}_q, \mathcal{A}_q$ become $\check{f}(y), \eta_{\pm}, W, A$, respectively, where

$$\begin{aligned} \check{f}(y) &:= f(x) \quad \text{with } x = y^2 \quad ; \\ (\eta_{\pm} f)(x) &:= \check{f}(y \pm \frac{i}{2}) \quad , \\ (Wf)(x) &:= \frac{1}{2yi}(\eta_+ f - \eta_- f)(x) \quad , \\ (Af)(x) &:= \frac{1}{2}(\eta_+ f + \eta_- f)(x). \end{aligned}$$

The above divided difference operator W is called the Wilson operator [24]. We have the relation

$$W(fg) = (Wf)(Ag) + (Af)(Wg).$$

Analogous to the q -Sturm-Liouville problem (2.5), we consider the following difference equation

$$\frac{1}{w(x)} W(p(x)Wf)(x) = r(x)f(x) \quad ,$$

which is equivalent to the Sturm-Liouville problem in the form,

$$\Pi(x)W^2 f(x) + \Phi(x)(AWf)(x) = r(x)f(x), \quad (6.1)$$

where Π, Φ are the functions defined by

$$\Pi(x) = \frac{1}{w(x)} Ap(x), \quad \Phi(x) = \frac{1}{w(x)} Wp(x). \quad (6.2)$$

For our purpose with reason which will be clearer later on, we seek polynomial solutions $f(x)$ to (6.1), but $\Pi(x), \Phi(x), r(x)$ are rational functions with the same degree constraints as in (2.10). From the relations

$$\begin{aligned} AWf(x) &= \frac{1}{i(4y^2+1)} \left\{ (y - \frac{i}{2})\eta_+^2 - (y + \frac{i}{2})\eta_-^2 + i \right\} f(x); \\ W^2 f(x) &= \frac{-1}{y(4y^2+1)} \left\{ (y - \frac{i}{2})\eta_+^2 + (y + \frac{i}{2})\eta_-^2 - 2y \right\} f(x), \end{aligned}$$

it follows that if $f(x_0) = 0$ for $x_0 = y_0^2$, then

$$\left(\frac{\eta_+^2 f}{\eta_-^2 f} \right) (x_0) = \frac{-(y_0 + \frac{i}{2})(\Pi(x_0) - \Phi(x_0)y_0 i)}{(y_0 - \frac{i}{2})(\Pi(x_0) + \Phi(x_0)y_0 i)}. \quad (6.3)$$

For a degree n polynomial $f(x)$ with roots x_j for $1 \leq j \leq n$, and let $x = y^2$, $x_j = y_j^2$, that is

$$f(x) = \gamma \prod_{j=1}^n (x - x_j) = \gamma \prod_{j=1}^n (y^2 - y_j^2), \quad \gamma \neq 0.$$

Then

$$\eta_{\pm}^2 f(x_k) = \gamma \prod_{j=1}^n (y_k - y_j \pm i)(y_k + y_j \pm i).$$

By (6.3), y_j 's satisfy the following system of equations,

$$\frac{-(y_k + \frac{i}{2})(\Pi(x_k) - y_k i \Phi(x_k))}{(y_k - \frac{i}{2})(\Pi(x_k) + y_k i \Phi(x_k))} = \prod_{j=1}^n \frac{(y_k - y_j + i)(y_k + y_j + i)}{(y_k - y_j - i)(y_k + y_j - i)}, \quad 1 \leq k \leq n,$$

or equivalently,

$$\frac{\Pi(x_k) - y_k i \Phi(x_k)}{\Pi(x_k) + y_k i \Phi(x_k)} = \prod_{j \neq k, j=1}^n \frac{(y_k - y_j + i)(y_k + y_j + i)}{(y_k - y_j - i)(y_k + y_j - i)}, \quad 1 \leq k \leq n. \quad (6.4)$$

We now consider the equation (6.1) which arises from (4.3) by letting $q \rightarrow 1$. In the notation of the q -gamma function [2], [9]

$$\Gamma_q(y) = \frac{(1-q)^{1-y}(q; q)_{\infty}}{(q^y; q)_{\infty}},$$

we make the identification

$$\frac{1}{(a_j e^{i\theta}, a_j e^{-i\theta}; q)_{\infty}} = \frac{\Gamma_q(-s_j - iy) \Gamma_q(-s_j + iy)}{(1-q)^{2+2s_j} (q; q)_{\infty}^2}, \quad a_j = e^{-s_j}.$$

Note the limiting property $\lim_{q \rightarrow 1} \Gamma_q(y) = \Gamma(y)$, for a proof see Appendix I in [1]. The limiting weight function (4.1) has the following expression:

$$w(x, \vec{a}) dx = \frac{(1 - q^{\frac{N}{2}})^2 (q^{\frac{N}{2}}; q^{\frac{N}{2}})_{\infty}^2 \prod_{l=1}^{2N} \Gamma_q(-s_l - iy) \Gamma_q(-s_l + iy) \log q}{(1-q)^{4N+2} \sum_j s_j (q; q)_{\infty}^{4N} (-iNy) \Gamma_{q^{\frac{N}{2}}} (iNy)} \times \frac{\sin \theta}{\sin \frac{N\theta}{2}} dy.$$

The fact $\lim_{\theta \rightarrow 0} \frac{\sin \theta}{\sin(N\theta/2)} = 2/N$ identifies the following weight function as the one corresponding to $q = 1$,

$$w(x, \vec{s}) = \left| \frac{\prod_{l=1}^{2N} \Gamma(-s_l + iy)}{\Gamma(iNy)} \right|^2. \quad (6.5)$$

Consequently the function $p(x)$ in the Sturm-Liouville problem (6.1) is given by

$$p(x) = w(x, \vec{s} - \frac{1}{2}) \quad \frac{1}{2} := (\frac{1}{2}, \dots, \frac{1}{2}).$$

The corresponding functions in in (6.2) will be denoted by

$$\Pi(x; \vec{a}) = \frac{1}{w(x, \vec{s})} A w(x, \vec{s} - \frac{1}{2}), \quad \Phi(x; \vec{a}) = \frac{1}{w(x, \vec{s})} W w(x, \vec{s} - \frac{1}{2}).$$

Theorem 6.1 For a given $\vec{s} = (s_1, \dots, s_{2N})$ with an even N , denote ς_j the j -th elementary symmetric function of s_i 's for $0 \leq j \leq 2N$, ($\varsigma_0 := 1$). Then $\Pi(x; \vec{a}), x\Phi(x; \vec{a})$ are the polynomials of x of degree at most N with following expressions,

$$\begin{aligned}\Pi(x; \vec{a}) &= (-1)^{\frac{N}{2}} \{x^N + \sum_{j=0}^{N-1} (-1)^j (\frac{1}{2}\varsigma_{2j+1} - \varsigma_{2j+2}) x^{N-j-1}\}, \\ x\Phi(x; \vec{a}) &= (-1)^{\frac{N}{2}} \{\sum_{j=0}^{N-1} (-1)^j (\frac{1}{2}\varsigma_{2j} - \varsigma_{2j+1}) x^{N-j-1} + \frac{1}{2}\varsigma_{2N}\}.\end{aligned}$$

The roots, $x_k = y_k^2$, $k = 1, \dots, n$, of a degree n polynomial solution $f(x)$ of the Sturm-Liouville problem (6.1) satisfy the following Bethe Ansatz type relation,

$$\frac{y_k - \frac{i}{2}}{y_k + \frac{i}{2}} \prod_{l=1}^{2N} \frac{y_k + s_l i}{y_k - s_l i} = \prod_{j \neq k, j=1}^n \frac{(y_k - y_j + i)(y_k + y_j + i)}{(y_k - y_j - i)(y_k + y_j - i)}, \quad 1 \leq k \leq n. \quad (6.6)$$

Proof. It is easy to see that

$$\begin{aligned}\eta_+ w(x, \vec{s} - \frac{1}{2}) &= \frac{\prod_{j=1}^{2N} \Gamma(-s_j - iy + 1) \Gamma(-s_j + iy)}{\Gamma(-iNy + \frac{N}{2}) \Gamma(iNy - \frac{N}{2})}, \\ \eta_- w(x, \vec{s} - \frac{1}{2}) &= \frac{\prod_{j=1}^{2N} \Gamma(-s_j - iy) \Gamma(-s_j + iy + 1)}{\Gamma(-iNy - \frac{N}{2}) \Gamma(iNy + \frac{N}{2})}.\end{aligned}$$

The functional equation of the Gamma function, $\Gamma(z+1) = z\Gamma(z)$, establishes the explicit representations for Π and Φ ,

$$\begin{aligned}\Pi(x; \vec{a}) &= \frac{(-1)^{\frac{N}{2}}}{2y} \{(y + \frac{i}{2}) \prod_{j=1}^{2N} (y - is_j) + (y - \frac{i}{2}) \prod_{j=1}^{2N} (y + is_j)\} \\ &= (-1)^{\frac{N}{2}} \{\sum_{j=0}^N (-1)^j \varsigma_{2j} x^{N-j} + \frac{1}{2} \sum_{j=0}^{N-1} (-1)^j \varsigma_{2j+1} x^{N-j-1}\} \\ &= (-1)^{\frac{N}{2}} \{x^N + \sum_{j=0}^{N-1} (-1)^j (\frac{1}{2}\varsigma_{2j+1} - \varsigma_{2j+2}) x^{N-j-1}\} \\ \Phi(x; \vec{a}) &= \frac{(-1)^{\frac{N}{2}}}{2y^2 i} \{(y + \frac{i}{2}) \prod_{j=1}^{2N} (y - is_j) - (y - \frac{i}{2}) \prod_{j=1}^{2N} (y + is_j)\}; \\ &= (-1)^{\frac{N}{2}} \{\sum_{j=0}^{N-1} (-1)^{j+1} \varsigma_{2j+1} x^{N-j-1} + \frac{1}{2} \sum_{s=0}^N (-1)^j \varsigma_{2j} x^{N-j-1}\} \\ &= (-1)^{\frac{N}{2}} \{\sum_{j=0}^{N-1} (-1)^j (\frac{1}{2}\varsigma_{2j} - \varsigma_{2j+1}) x^{N-j-1} + \frac{1}{2}\varsigma_{2N} x^{-1}\}.\end{aligned}$$

Hence we obtain the expressions of $\Pi(x; \vec{a}), x\Phi(x; \vec{a})$. By the first expressions for $\Pi(x; \vec{a}), \Phi(x; \vec{a})$ in terms of y in the above right hand sides, one can easily derive the following identities:

$$\Pi(x; \vec{a}) - \Phi(x; \vec{a}) y i = \frac{(-1)^{\frac{N}{2}}}{y} (y - \frac{i}{2}) \prod_{j=1}^{2N} (y + is_j), \quad \Pi(x; \vec{a}) + \Phi(x; \vec{a}) y i = \frac{(-1)^{\frac{N}{2}}}{y} (y + \frac{i}{2}) \prod_{j=1}^{2N} (y - is_j),$$

hence

$$\frac{\Pi(x; \vec{a}) - \Phi(x; \vec{a})yi}{\Pi(x; \vec{a}) + \Phi(x; \vec{a})yi} = \frac{y_k - \frac{i}{2}}{y_k + \frac{i}{2}} \prod_{j=1}^{2N} \frac{y + s_j i}{y - s_j i}.$$

By the above relation and (6.4), we obtain (6.6). \square

Remark. For the Bethe Ansatz equations (6.6) with N odd, one can reduce the problem to the above theorem for some even N' by adding certain zero-value s_j 's. By the similar method, one enables to apply the above theorem to Bethe Ansatz problem of the following type with $s_1, \dots, s_M \in \mathbf{C}$ and $M \in \mathbf{N}$,

$$\prod_{l=1}^M \frac{y_k + s_l i}{y_k - s_l i} = \prod_{j \neq k, j=1}^n \frac{(y_k - y_j + i)(y_k + y_j + i)}{(y_k - y_j - i)(y_k + y_j - i)}, \quad 1 \leq k \leq n, \quad (6.7)$$

\square

For a positive half-integer s , it is known that the spin s XXX model of an even size L with the periodic boundary condition has the following Bethe Ansatz equations:

$$\left(\frac{\lambda_k + si}{\lambda_k - si} \right)^L = \prod_{j=1, j \neq k}^l \frac{\lambda_k - \lambda_j + i}{\lambda_k - \lambda_j - i}, \quad \lambda_k \in \mathbf{C}, \quad k = 1, \dots, l. \quad (6.8)$$

In the antiferromagnetic case, the ground state is on the sector $l = \frac{L}{2}$; conjecturally there is the unique real solution of the Bethe Ansatz equations. Note that $\{-\lambda_j\}_{j=1}^l$ is a solution of (6.8) whenever $\{\lambda_j\}_{j=1}^l$ is a solution. Hence for the ground state, the roots λ_j s are expected to be real and invariant under the sign-change (up to permutation of the indices j). Having this ground state conjecture in mind, we now consider a general problem of (6.8) for $l \equiv \frac{L}{2} \pmod{2}$ with roots invariant under the change of sign, $\lambda_j \mapsto -\lambda_j$, i.e., λ_j s with the following form:

$$L = 4M + 2, \quad \{\lambda_j\}_{j=1}^l = \{0, \pm y_1, \dots, \pm y_n\}; \quad (6.9)$$

$$L = 4M, \quad \{\lambda_j\}_{j=1}^l = \{\pm y_1, \dots, \pm y_n\}. \quad (6.10)$$

In this situation, one can link the Bethe Ansatz equations (6.8) of XXX model to the Sturm-Liouville problem previously discussed in this section. In the case (6.9), the relation (6.8) becomes

$$\frac{(y_k - \frac{i}{2})(y_k - i)(y_k + si)^{4M+2}}{(y_k + \frac{i}{2})(y_k + i)(y_k - si)^{4M+2}} = \prod_{j=1, j \neq k}^n \frac{(y_j - y_k + i)(y_j + y_k + i)}{(y_j - y_k - i)(y_j - y_k + i)}, \quad y_k \in \mathbf{C} \setminus \{0\}, \quad k = 1, \dots, n,$$

in which case, we set the N , s_j 's in Theorem 6.1 as follows:

$$\begin{aligned} L = 4M + 2, \quad s \neq 1: \quad N = 2M + 2, \quad s_1 = 0, \quad s_2 = -1, s_3 = \dots = s_{2N} = s, \\ s_{2N} = 0, \quad s_j = \binom{2N-2}{j} s^j - \binom{2N-2}{j-1} s^{j-1}, \quad 0 \leq j \leq 2N - 1; \\ s = 1: \quad N = 2M + 1, \quad s_1 = 0, \quad s_2 = \dots = s_{2N} = 1, \\ s_{2N} = 0, \quad s_j = \binom{2N-1}{j} \quad 0 \leq j \leq 2N - 1. \end{aligned} \quad (6.11)$$

In the case (6.10), one has

$$\frac{(y_k - \frac{i}{2})(y_k + si)^{4M}}{(y_k + \frac{i}{2})(y_k - si)^{4M}} = \prod_{j=1, j \neq k}^n \frac{(y_j - y_k + i)(y_j + y_k + i)}{(y_j - y_k - i)(y_j - y_k + i)}, \quad y_k \in \mathbf{C} \setminus \{0\}, \quad k = 1, \dots, n, \quad (6.12)$$

in which case, N, s_j in Theorem 6.1 are given by

$$L = 4M, \quad N = 2M, \quad s_1 = \dots = s_{2N} = s, \quad s_j = \binom{2N}{j} s^j \quad \text{for } 0 \leq j \leq 2N. \quad (6.13)$$

For both situations, the relations are of the form (6.7) for suitable s_l 's. Note that the non-zero condition of y_k s in (6.9), (6.10) for the corresponding polynomial solution $f(x)$ of (6.1) requires one further constraint, namely $f(0) \neq 0$. The ground state of antiferromagnetic spin s XXX model of size L is governed by the real root solution of the above equations for $n = \frac{L}{2}$.

We now consider the case $s = \frac{1}{2}$ and discuss some mathematical problems relevant to the physics of the system. The Hamiltonian is given by H_{XXX} in (1.4). We will discuss the Bethe Ansatz equations (6.12) with $s = \frac{1}{2}$ in (6.11) (6.13). To illustrate the mathematical content connecting to the Bethe Ansatz equations for the Hamiltonian H_{XXX} , we consider the case $L = 2, 4$. For $L = 2$ in (6.9), by

$$|\Gamma(iy)|^2 = \frac{\pi}{y \sinh \pi y}, \quad \left| \Gamma\left(\frac{-1}{2} + iy\right) \right|^2 = \frac{4\pi}{(4y^2 + 1) \cosh \pi y},$$

the weight function is expressed by

$$w(x) = \left| \frac{\Gamma(iy)\Gamma(1+iy)\Gamma(\frac{-1}{2}+iy)^2}{\Gamma(2iy)} \right|^2 = \frac{(2\pi)^3 y}{(x + \frac{1}{4})^2 \sinh 2\pi y}.$$

By (6.11), the corresponding Sturm-Liouville problem (6.1) is governed by the equation

$$(8x^2 + 6x + 1)W^2 f(x) + (4x + 1)AW f(x) = \lambda f(x)$$

with $\lambda = 4n(2n - 1)$ except $n = 1$, in which case $\lambda = 4$. For $L = 4$ in (6.9), by (6.13) we have the following weight function and the Sturm-Liouville problem,

$$w(x) = \left| \frac{\Gamma(\frac{-1}{2} + iy)^4}{\Gamma(2iy)} \right|^2 = \frac{4\pi^3 y \sinh \pi y}{(x + \frac{1}{4})^4 \cosh^3 \pi y}$$

$$-x(32x^2 - 16x - 6)W^2 f(x) + (48x^2 + 8x - 1)AW f(x) = (\lambda x + \mu)f(x)$$

with $\lambda = -16n(2n - 1)$ except $n = 1$, in which case $\lambda = 48$. For $n = 1$, we have $\mu = 4$ and $f(x) = x + \frac{1}{4}$. Note that due to the parameters in the above weight functions, the Sturm-Liouville problems we encounter here does not make the Wilson polynomials orthogonal, as in [4]. However, our empirical computation for the case $L = 2$ has indicated that the $f(x)$'s are real polynomials with $f(0) \neq 0$. For the general size L , the weight function of the Sturm-Liouville problem connecting to XXX model in the context of discussions in this section has

the following expressions:

$$\begin{aligned}
L = 4M + 2, \quad w(x) &= \left| \frac{\Gamma(iy)\Gamma(1+iy)\Gamma(\frac{-1}{2}+iy)^L}{\Gamma((\frac{L}{2}+1)iy)} \right|^2 = \frac{(\frac{L}{2}+1)\pi^{L+1}y \sinh(\frac{L}{2}+1)\pi y}{(x+\frac{1}{4})^L \sinh^2 \pi y \cosh^L \pi y}, \\
L = 4M, \quad w(x) &= \left| \frac{\Gamma(\frac{-1}{2}+iy)^L}{\Gamma(\frac{L}{2}iy)} \right|^2 = \frac{\frac{L}{2}\pi^{L-1}y \sinh \frac{L}{2}\pi y}{(x+\frac{1}{4})^L \cosh^L \pi y}.
\end{aligned}$$

Nevertheless a sound mathematical treatment of their corresponding Sturm-Liouville equations appears still lacking now, and it remains a difficult task to obtain substantial knowledge incorporating the physical applications associated to XXX model. However The quest of a such mathematical theory would be a necessary one in order to understand the essential features of the Bethe Ansatz equations for the Heisenberg XXX spin chain.

7 Conclusions and Perspectives

In this paper we have provided a one to one correspondence between polynomial solutions to Sturm-Liouville type equation involving the Askey-Wilson operator and solutions of the algebraic Bethe Ansatz equations of XXZ and XXX models. We have also started a preliminary study of the mathematical problems arising from the physics of the Bethe Ansatz. In doing so we have reduced the nonlinear problem of solving the Bethe Ansatz equations to the linear problem of finding polynomial solutions to certain linear second order equations in terms of the Askey-Wilson or Wilson operator. Thus the physics of XXZ model has indeed raised some mathematical questions which demand the need for a systematic mathematical development in the theory of the corresponding q -difference equations. The mathematical solution of those questions will lead to a better understanding of some interesting physical quantities of XXZ and XXX models. We intend to continue this study in future and partial results obtained so far are indeed very promising.

Acknowledgments M. Ismail acknowledges financial support from Liu Bie Ju Center of Mathematical Sciences in Hong Kong, and the Academia Sinica of Taiwan, where this work started. This paper was partially supported by NSF grant DMS 99-70865 and NSC grant 89-2115M001037 of Taiwan.

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